Basic Research Needs

Workshop on Materials Under Extreme Environments

Jeff Wadsworth (Oak Ridge)

Russell Hemley (Carnegie Institution)

George Crabtree (Argonne)

Special thanks: Michelle Buchanan

Workshop on Hard Materials
Brookhaven National Laboratory
February 6, 2008

The Basic Research Needs Workshops

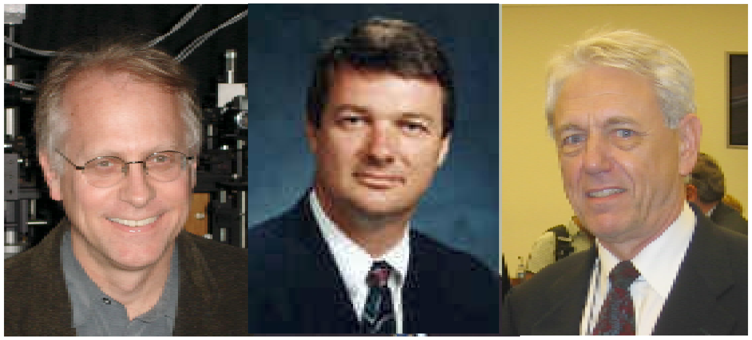
Basic Research in Support of the DOE Missions

http://www.sc.doe.gov/bes/reports/list.html

- **Basic Research Needs to Assure a Secure Energy Future**
  BESAC Workshop, October 21–25, 2002
  The foundation workshop that set the model for the focused workshops that follow
- **Basic Research Needs for the Hydrogen Economy**
  BES Workshop, May 13–15, 2003
- **Basic Research Needs for Solar Energy Utilization**
  BES Workshop, April 18–21, 2005
- **Basic Research Needs for Superconductivity**
  BES Workshop, May 8–10, 2006
- **Basic Research Needs for Solid-state Lighting**
  BES Workshop, May 22–24, 2006
- **Basic Research Needs for Advanced Nuclear Energy Systems**
  BES Workshop, July 31–August 3, 2006
- **Basic Research Needs for the Clean and Efficient Combustion of 21st Century Transportation Fuels**
  BES Workshop, October 30–November 1, 2006
- **Basic Research Needs for Electrical Energy Storage**
  BES Workshop, April 2007
- **Basic Research Needs for Geosciences: Scientific Challenges for Measurement, Monitoring, and Verification**
  BES Workshop, Spring 2007
- **Basic Research Needs for Materials Under Extreme Environments**

Basic Research Needs Workshop on Materials Under Extreme Environments

June 11-14, 2007



Workshop Chair:
Jeff Wadsworth (ORNL)

Associate Chairs:
Russell Hemley (Carnegie Institution)
George Crabtree (ANL)

Plenary Speakers

Pat Dehmer, BES	Bob Schoenlein, LBNL
Sam Baldwin, EERE	Larry Fried, LLNL
Robert Romanosky, FE	Neil Ashcroft, Cornell
Christopher Deeney, NNSA	Bob Laughlin, Stanford

Panel Leads

Energetic photon/particle flux
Roger Falcone (ALS), Ian Robertson (UIUC)

Chemical extremes
John Stringer (EPRI, ret), Peter Tortorelli (ORNL)

Thermomechanical extremes
Rusty Gray (LANL), Malcolm Nicol (UNLV)

Electromagnetic extremes
Jane Lehr (Sandia), Stan Tozer (NHMFL)

Cross cutting science
Tomas de la Rubia (LLNL), John Sarrao (LANL)

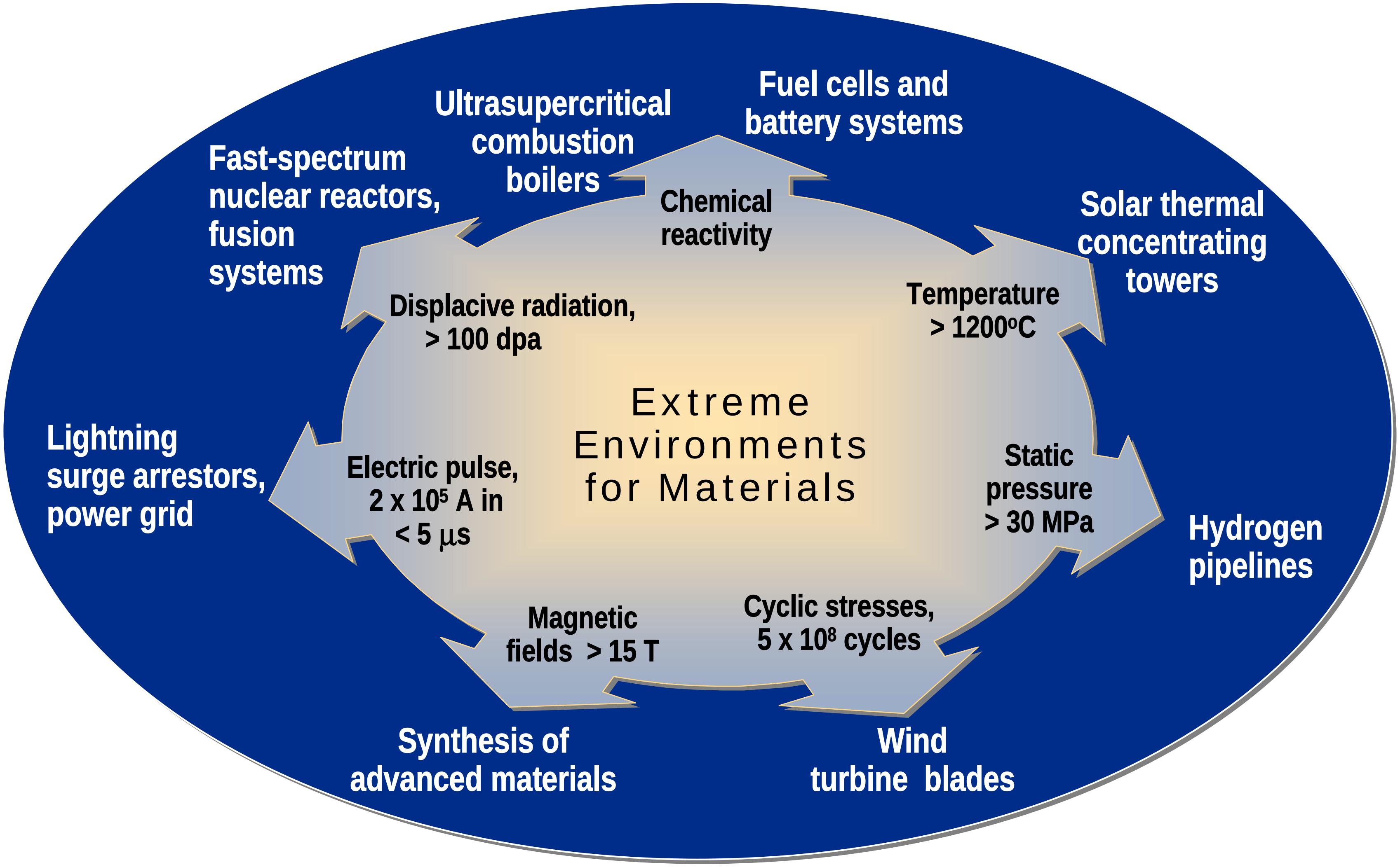
Tim Fitzsimmons: BES Coordinator

Charge

Identify basic research needs and opportunities in materials under extreme environments encountered in energy generation, conversion and utilization processes, with a focus on new, emerging and scientifically challenging areas that have the potential to significantly impact science and technology.

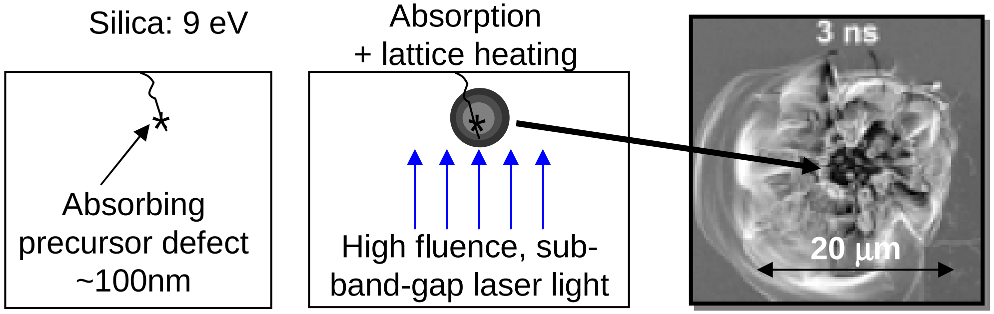
160 participants
Academia, Industry, National Labs
Basic and Applied DOE Energy Offices

Extreme Energy Environments



Energetic Photon / Particle Damage

Photon Damage on Polished Glass



Best performance today - 20 J/cm^3

Intrinsic limit - 200 J/cm^3

Initiated by single nanoscale defects

Complex damage trajectory to failure

Research Directions

In situ, real time, atomic scale damage characterization

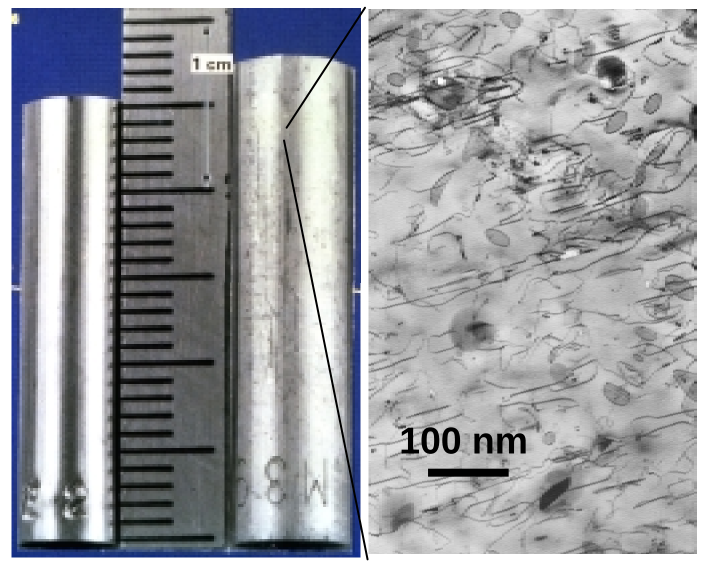
Capture multiscale damage dynamics

Defect-free or defect tolerant materials

Technology Drivers

- Next generation nuclear reactors
- MW lasers for fusion
- Microelectronic sensors for active environments

Neutron Damage on Stainless Steel



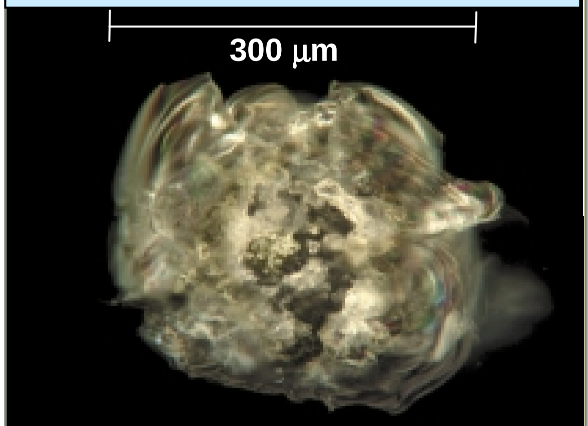
control 1.5 x 10^{23} n cm^{-2}

20% CW 316 stainless steel, 796 K

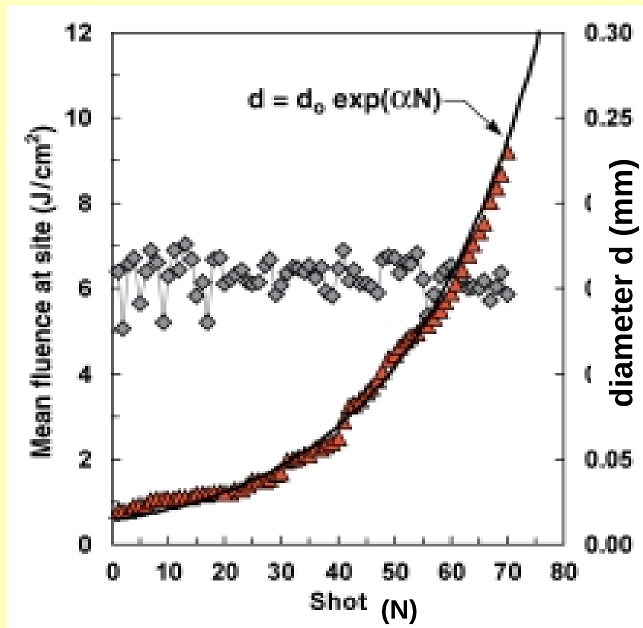
Laser-induced damage limits the performance of high power lasers

Laser-induced surface damage on SiO_2	Damage growth under repeated illumination	Growth exponent increases linearly with fluence

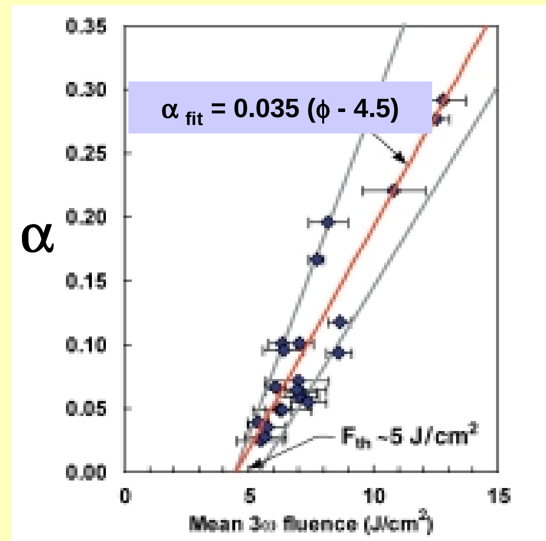
9 shots @ 10.5J/cm², 3ω, 10ns



- UV light produces exit-surface damage on high-value SiO_2 optics
- Optical quality of SiO_2 lenses degrades when too many damage sites are present



- The size of a damage site grows exponentially as a function of the number of laser shots

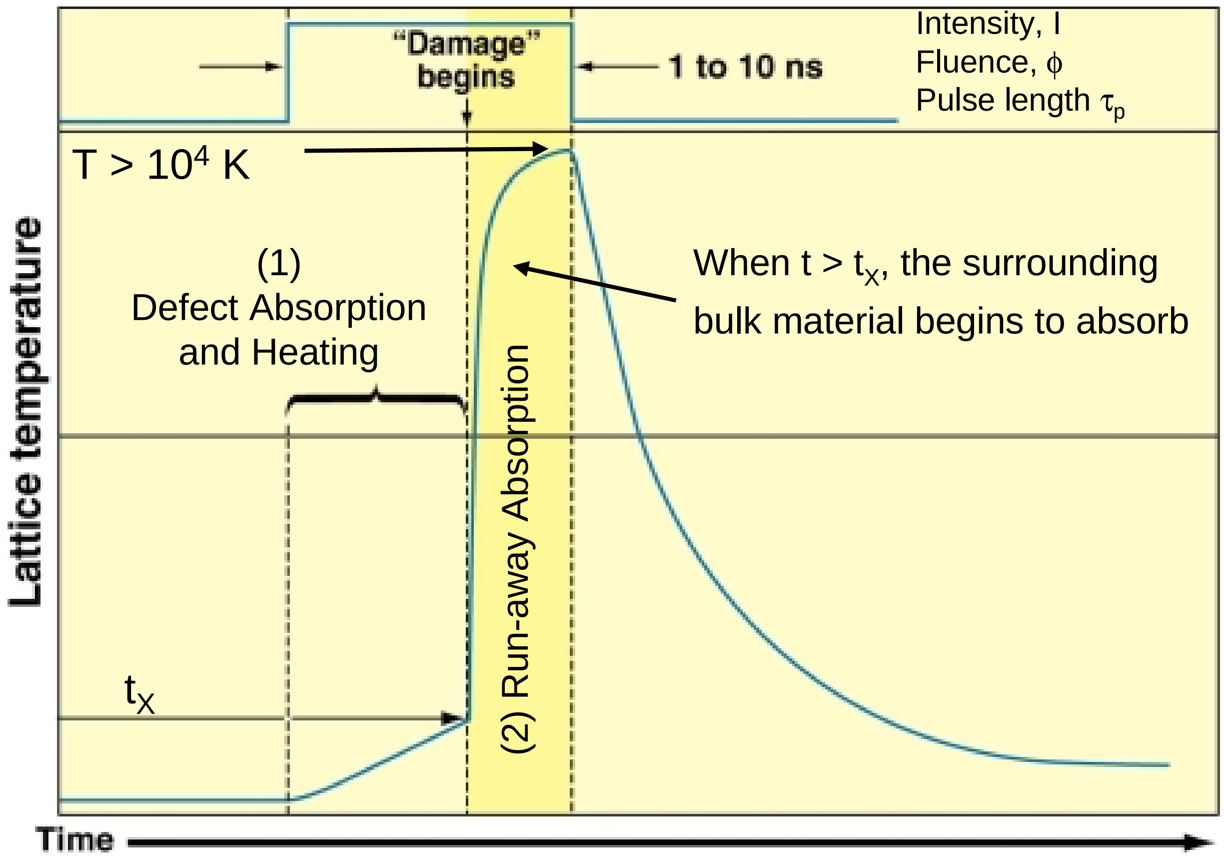


- At 0.3 µm (3ω) the fluence threshold for damage is: ***Φ ~ 5 J/cm²***
- Optics on NIF experiences a fluence of ***Φ ~ 8 J/cm²*** at 2 MJ

The development of damage-resistant optics would revolutionize materials research worldwide

Challenges: Understanding and Controlling Optical Damage

Optical damage occurs in a sequence of two steps



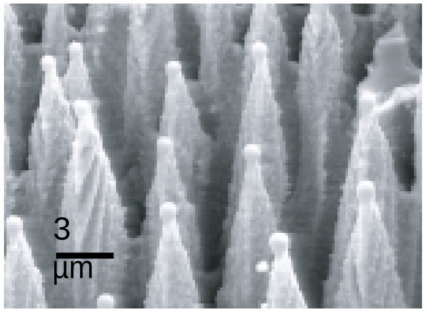
Which defects absorb sub-gap light and lead to damage?

How can we find them?

How can we control them?

- Imaging a damage event
- Measure temperature activated absorption
- Ab-initio models for temperature activated absorption
- Full hydrodynamics including absorption model and materials response

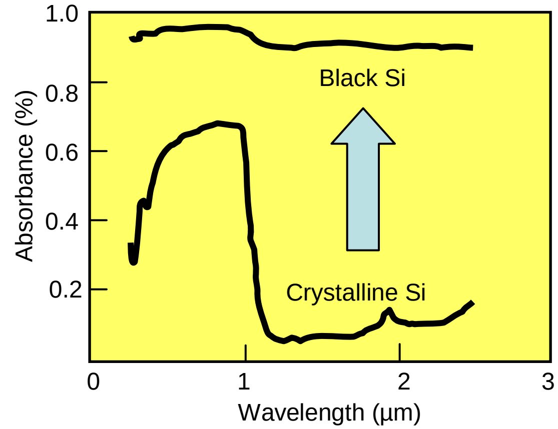
Flux Extremes: Synthesis of New Materials



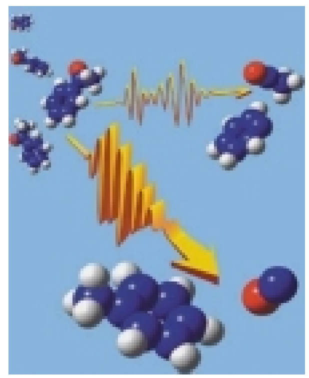
“Black Si”

fs laser-generated chalcogen-rich plasma

solar cells, photodiodes

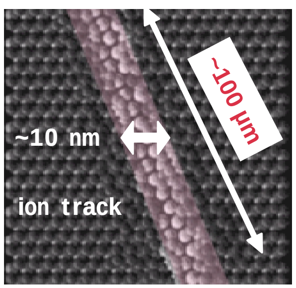


Intense, coherent pulses of THz electric fields control nuclear positions . . .

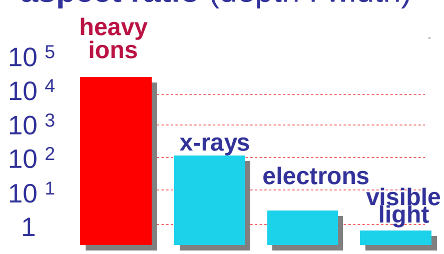


. . . and dictate chemical reaction pathways

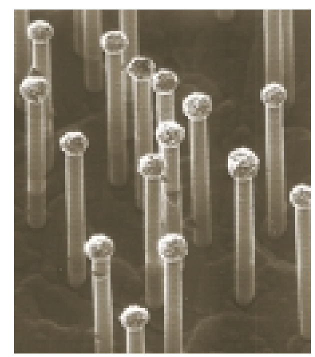
High aspect ratios with swift heavy ions



aspect ratio (depth : width)



single nanopore



nanowires

Chemically Reactive Extremes

High efficiency steam plants

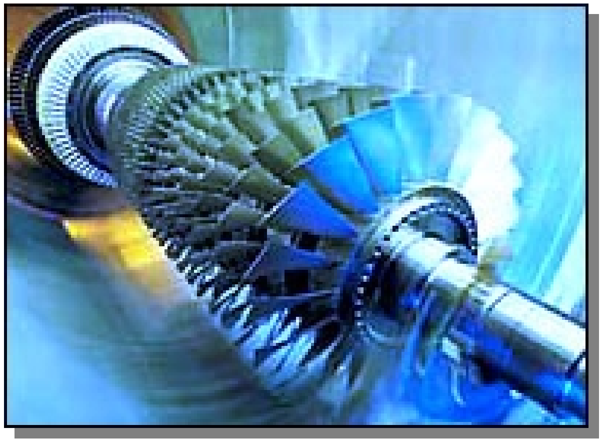
Next generation turbines

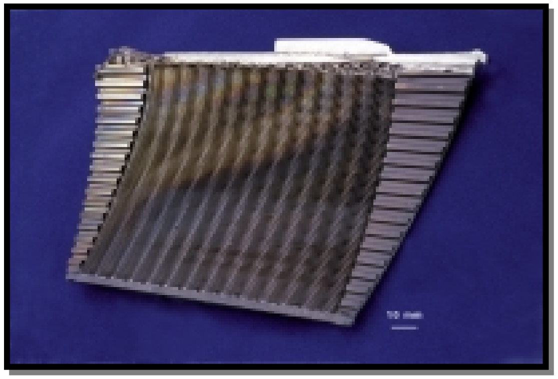
All types of fuel cells

Battery electrochemistry

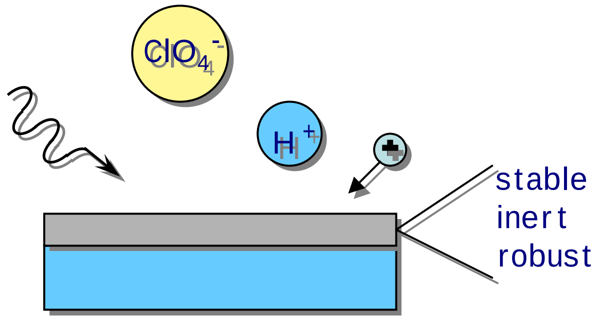
Nuclear power conversion

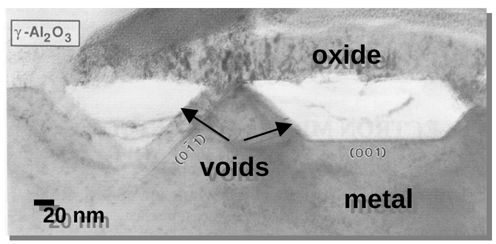
Thermochemical production of hydrogen





Controlling Reactive Environments





voids at buried interface

Research Directions

Atomic scale, real time, in situ measurements

Capture multiscale damage evolution

Multifunctional protective coatings

Nitrides, borides, carbides

Transform empirical data to predictive science

Protective oxide layer

Strongly bonded to substrate

Chemically inert to environment

Thermodynamically stable at all temperatures

Atomic scale defects trigger damage growth

Local chemical reactions

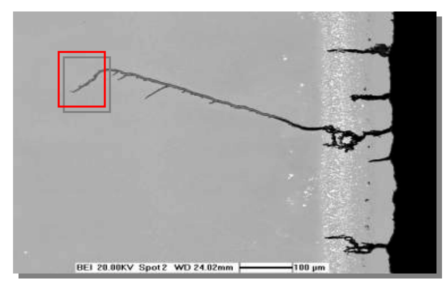
Internal stress

Defects form at exposed surface and buried interface

Complex damage trajectory

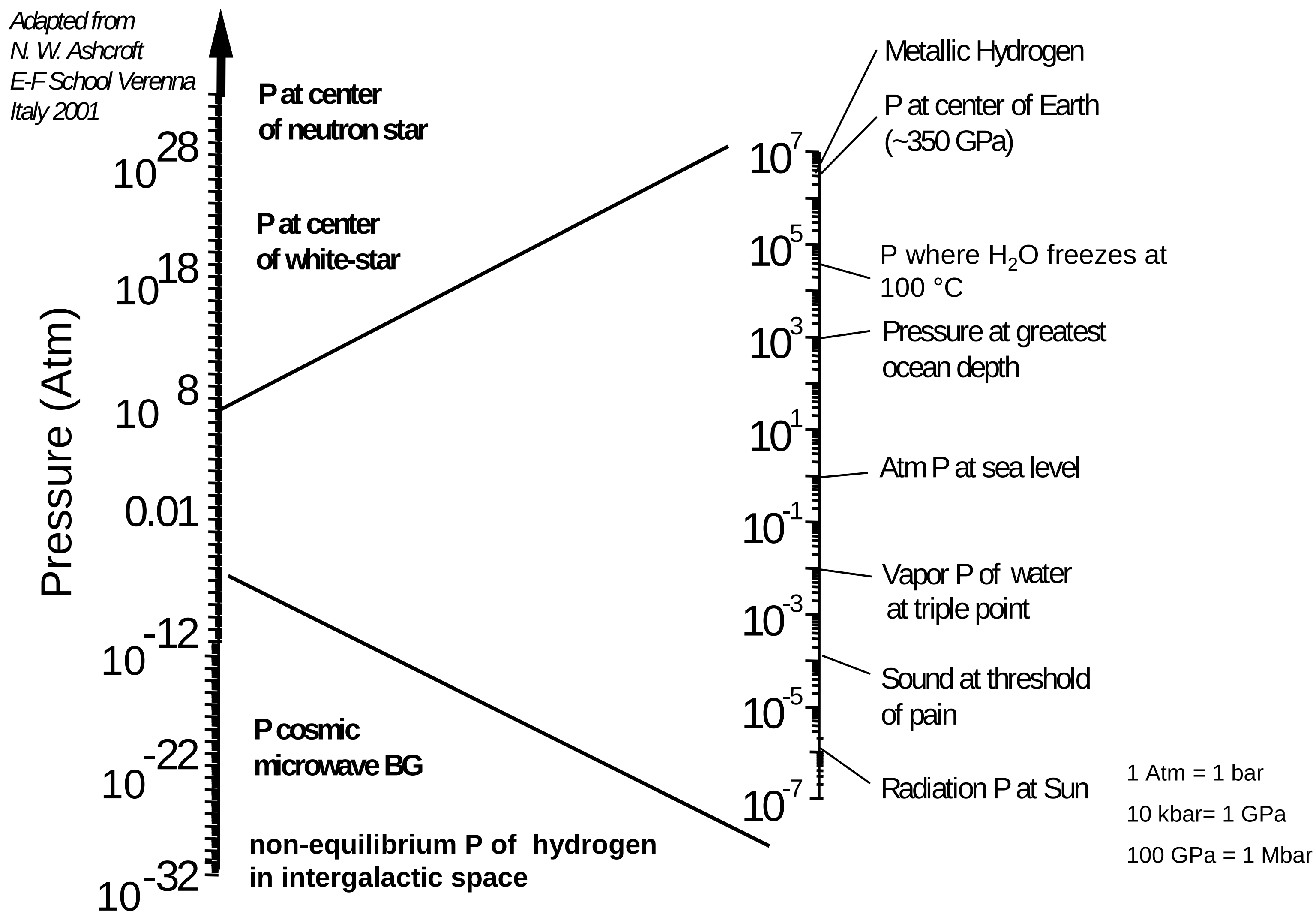
Many interacting degrees of chemical and mechanical freedom

Linked across many length and time scales



crack propagation from exposed surface

The Extreme Range of Pressure



Materials in Thermomechanical Extremes

Profusion of new structures at high pressure

Multiphase equation of state

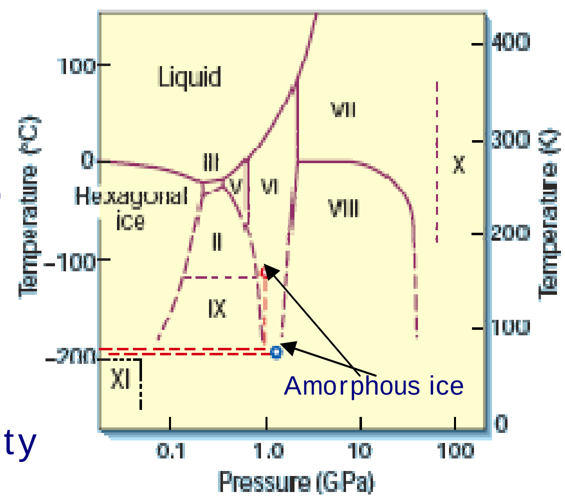
Maximum pressure rising for static, isentropic, and shock generation

Unconventional high pressure materials

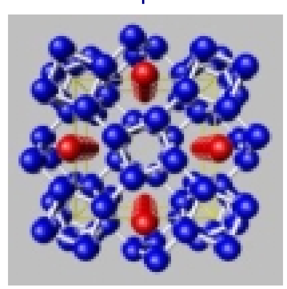
- Amorphous ice at 40% higher density
- Polymeric N, CO, and CO_2 - high energy density
- *Dynamic* pressure: C in cubic, hexagonal and amorphous diamond phases

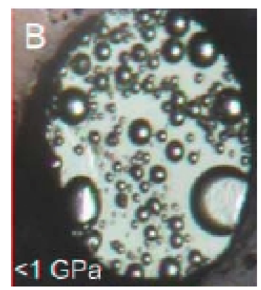
Recover high pressure phases to ambient, exploiting transformation barriers

Phase diagram of ice



Li under pressure





combined x-ray pressure-induced dissociation of water

Technology Drivers

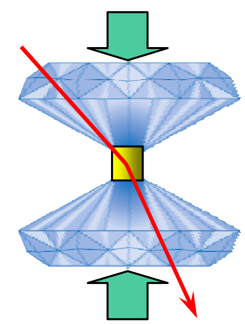
High temperature/strength materials for coal gasification

UltraSupercritical boilers and turbines

Next generation manufacturing technologies

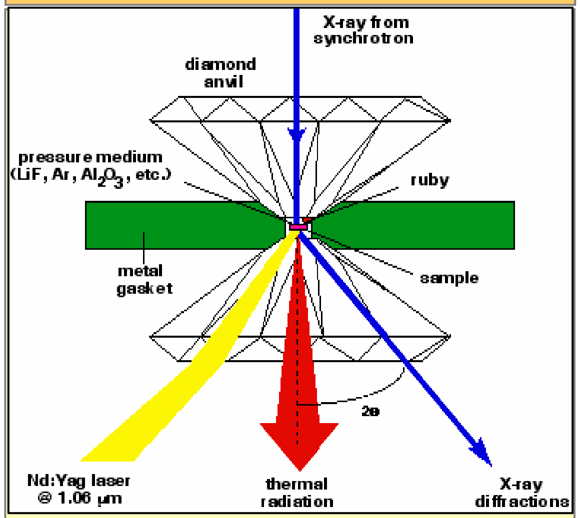
single crystal diamond by CVD

12 mm ~ 10 carat



Probing and Modeling Materials under High Static and Dynamic Pressure

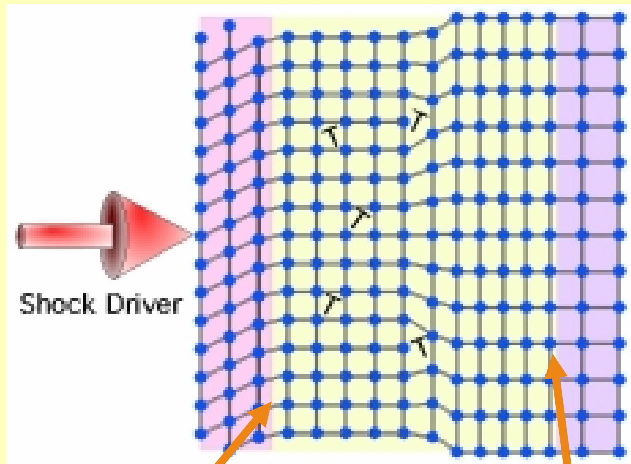
Static high-pressure research



Diamond anvil cell

- Isotherms
- Phase transitions
- EOS / melt
- Yield strength
- Elastic moduli

Dynamic high-pressure research

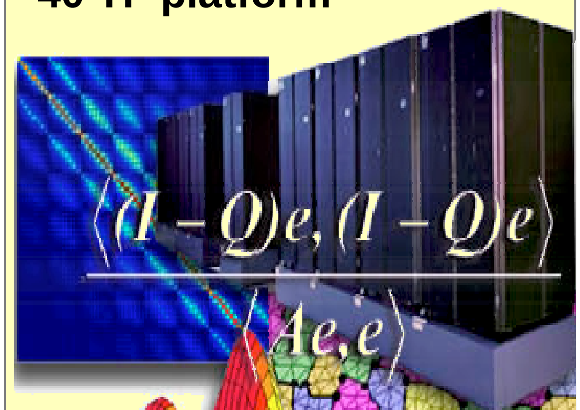


Transformation front Shock front

- Ultrafast science of dynamically driven systems —
- "catching reactions in the act"
  - Materials science
  - Chemistry
  - Biology

High-performance scientific computing

40 TF platform



- Multi-scale simulations of materials under extreme dynamic conditions:
  - Thermodynamic properties
  - Constitutive properties

Performing experiments and simulations at the same scale

Thermomechanical Challenges

Characterize high static and dynamic pressure phases

In situ experiments at BES x-ray, neutron and electron scattering and NNSA high energy facilities

Time evolution of structural phase transitions and role of defects

Chemical reaction dynamics of high energy materials

High pressure response of disordered materials

Raise the limits of high pressure static and dynamic generation

Electric Field Extremes

Electric field performance (MV/m)

1 Power cables

3 Lightning

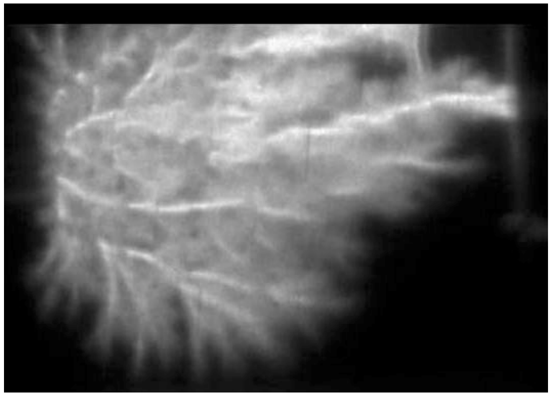
5 Saturn x-ray discharge machine

100 Peaking spark discharge

500 MEMS static charge

1000 microelectronics gate electrodes

Dielectric breakdown



performance limit for

power cables

high energy capacitors

motors and generators

microelectronics

10x below intrinsic limit

Trigger: atomic / nanoscale defect

Ultrafast, multiscale

Catastrophic failure

Research Directions

Ultrafast in situ characterization

Theoretical framework
- ultrafast dynamics
- multiscale modeling

New dielectric materials
- polymers
- nanofilled composites

Magnetic Field Extremes

Magnetic field limits

1 T permanent magnet

23 T superconducting (45 T hybrid dc resistive)

90 T pulsed (310 T destructive)

13 T cyclic (ITER – strength limit of steels)

500 T electron orbital radius ~ 1 nm

10^6 - 10^8 T neutron star

Higher fields ⇒ higher performance motors / generators

Limit to higher fields: strength of materials

Magnetic field: a thermodynamic variable

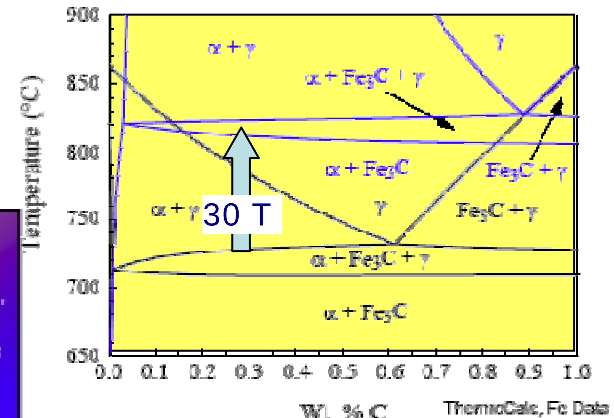
Like P or T, it accesses new phases of matter

Magnetic energies μH ~ 1.3 K/T

affects electronic correlations, not chemical bonds

localization, magnetism, superconductivity

mixing, formation, defects, diffusion barriers, elastic constants

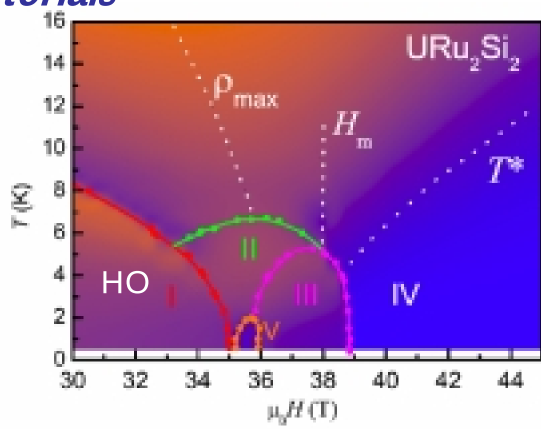


Fe-C alloy

Research Directions

Higher magnetic fields

In situ high field experiments at scattering sources



→ H > 500 T High Temperature Superconductors

Crosscutting Challenges

Experiments on the scale of the fundamental interactions

Atomic scale, in situ, real time characterization at user facilities

Theoretical and simulation framework for predicting and extrapolating performance

Capture complex multiscale phenomena and predict beyond accessible regimes

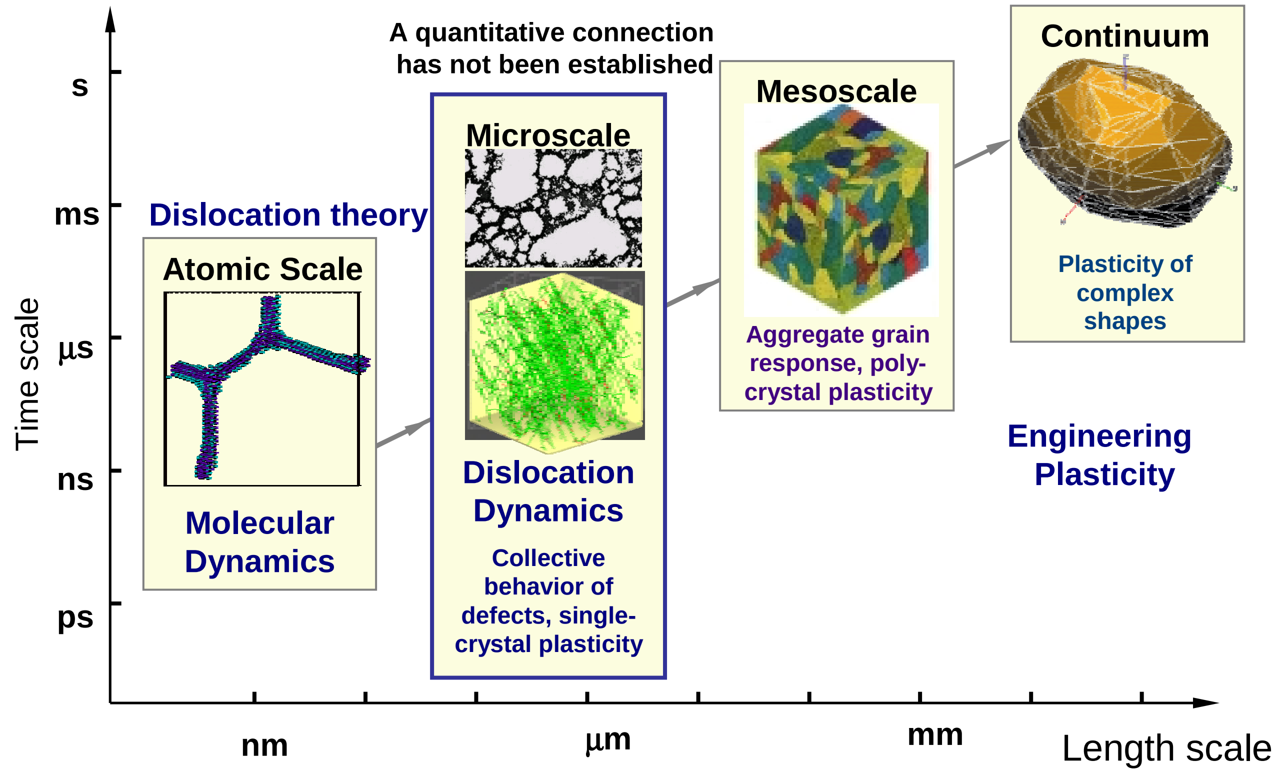
Design and synthesis of transformational materials

Control atomic structure and complex damage evolution

Extreme environments for materials design and synthesis

Photon / particle flux, chemical reactivity, thermomechanical, electromagnetic fields

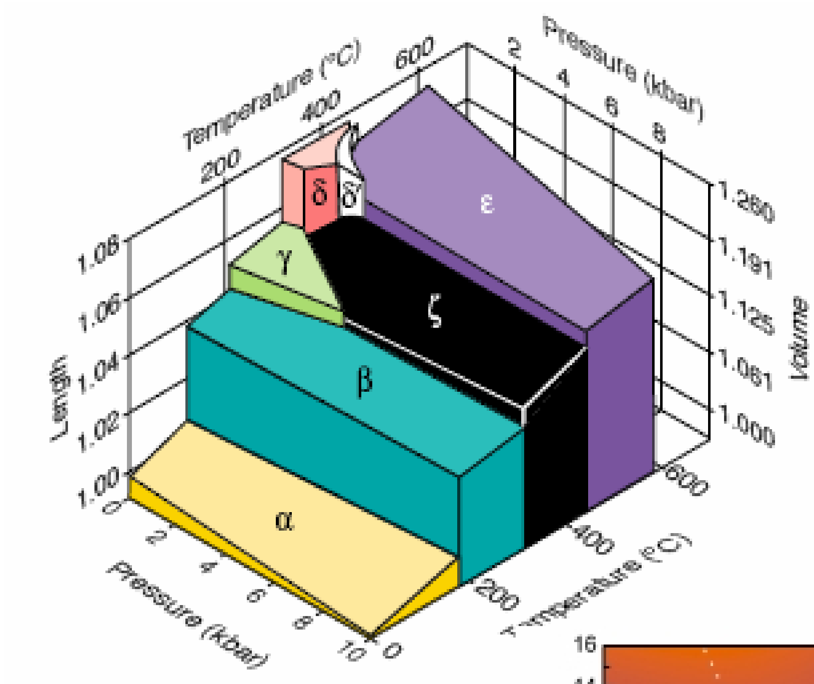
Multi-scale Simulation: a Cross-Cutting Challenge and Opportunity

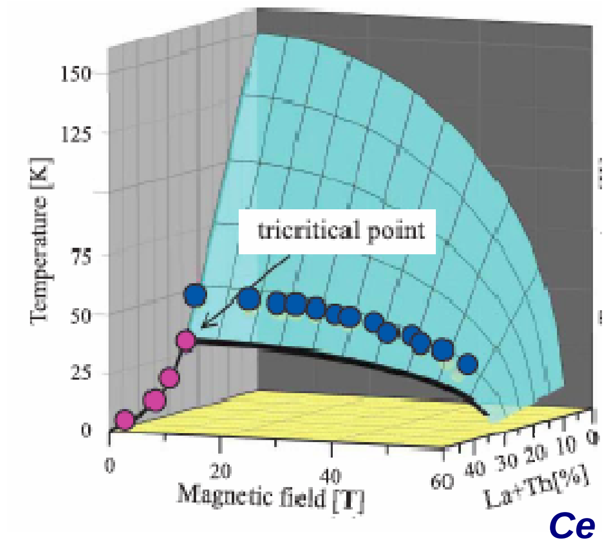


Today: manually connect the length and time scales

Tomorrow: self-assembled algorithms automatically adjust length and time scales

Multiple Extremes: Understanding Complexity on the Verge of Instability



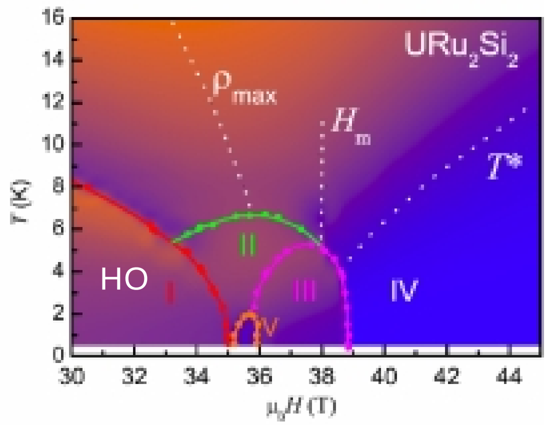


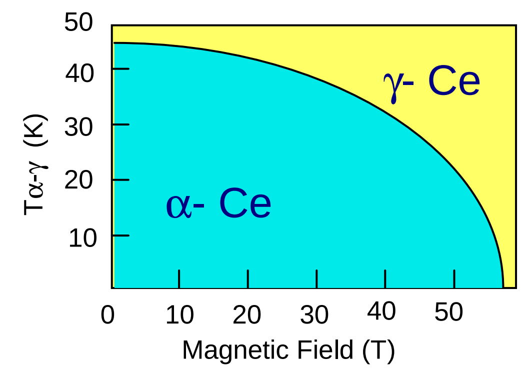
Ce

Highly correlated 4f electrons
Complex P-T-B-alloy phase diagram
Rich electronic behavior
$CeCu_2Si_2$ - heavy electron superconductor

Pu, U

Highly correlated 5f electrons
internal radiation
Complex P-T-B-alloy phase diagram
Rich electronic behavior
$PuCoGa_5$ - 18.5 K superconductor





Priority Research Directions

Control and synthesize materials with new properties using photon and particle beams

Design of materials with revolutionary tolerance to extreme photon and particle fluxes

Toward ideal surface stability

Controlling reaction dynamics at extremes

Novel materials by design - beyond what we know

Chemical and materials dynamics in complex systems

Disordered materials in the extreme

Fundamental processes of dielectric breakdown at the atomic level

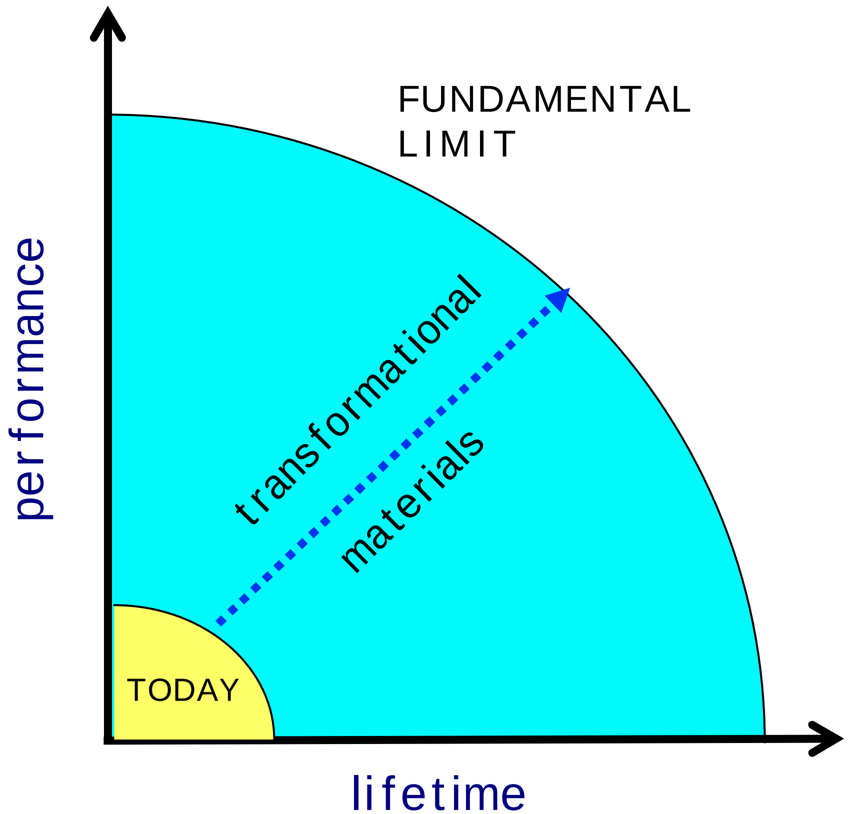
Achieving the quantum limit of extreme magnetic field

Materials Under Extreme Environments

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
▪ Dynamics of excitation and relaxation under extreme flux ▪ Fundamental limits of dielectric performance ▪ Bond-energy-charge relationships over relevant conditions ▪ Novel states of matter in extreme magnetic fields ▪ Complex chemistry and physics of degradation ▪ Multi-dimensional in-situ characterization tools ▪ Extreme environments as probes of materials behavior ▪ Self assembled multi-paradigm algorithms for understanding materials performance ▪ Atomic level understanding of dynamic behavior ▪ Fundamental knowledge of non-equilibrium systems ▪ Design and synthesis of transformational materials	▪ Achieving stable, non-reacting surfaces ▪ Exploit kinetic states far from equilibrium ▪ Mitigating materials degradation under extreme conditions ▪ Simulating and measuring dynamics at the same length and time scales ▪ Understanding dynamic behavior across interfaces ▪ Enabling a new generation of non-traditional materials for extreme environments ▪ Development of highly robust materials for extreme environments ▪ Harnessing extreme conditions to create new materials with revolutionary functionality	▪ Application of models and computational tools for system design and diagnostics for energy technologies requiring high strength and temperature ▪ Material evaluation and process development for radiation resistant materials for use in solar thermal, defense, nuclear reactors, and waste storage ▪ Improve long-term stability under extreme temperature, cyclic loads, pressure, chemical reactivity and electromagnetic field for energy generation and use ▪ Develop and apply novel materials processes and manufacturing technologies ▪ Proof of technology concepts with improved performance and reduced cost for use in extreme conditions	▪ Demonstrate energy production and utilization systems operating at high efficiency ▪ Support the establishment of domestic manufacturing capabilities for highly robust components and systems ▪ Development and deployment of reliable, high-capacity distribution and storage systems for centralized and distributed power sources ▪ Develop long-life, low-cost reliable, environmentally friendly recyclable processes for energy applications ▪ Computer validation of multifunctional materials performance for applications in extreme environments

Grand Challenge: Extreme Materials

Achieve the Fundamental Performance Limit



- Orders of magnitude improvement
- Realize the potential of unexplored extremes